Tetrachloro($^{13}C_2$)ethene

32488-49-6 | DTXSID10745778

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 170 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.88e-01

Confidence level: 7.31e-01

Nearest Neighbors from the Training Set

Image not found
Tetrachloroethylene
Measured: 251
Predicted: 170

Image not found
1,2-Dibromoethylene
Measured: 44.7
Predicted: 57.8

Image not found
Carbon tetrachloride
Measured: 70.8
Predicted: 69.4

Image not found
Chloroform
Measured: 39.8
Predicted: 50.3

Image not found
Chloropicrin
Measured: 61.7
Predicted: 61.7